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by

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16. ABSTRACT

A hybrid receptor model is a specified mathematical procedure which uses not only the ambient species concentration measurementsthat form the input data for a pure receptor model, but in addition source emission rates or atmospheric dispersion or transformation information characteristic of dispersion models. By utilizing more information hybrid receptor modeling promises improved source apportionment estimates or, more fundamentally, consideration of problems that are inaccessible in terms of classical receptor modeling. Two examples of hybrid receptor models are reviewed to illustrate the variety in possible approaches.

Some hybrid receptor modeling results are given for the comprehensive ambient-source meteorological data base collected at Deep Creek, Maryland, during summer 1983. By using source and ambient measurements of selenium about 33% of the sulfate impact at the receptor site during a day-time period can be associated with emissions from a coal-fired power plant 50 KM upwind.

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1. INTRODUCTION

Dispersion trajectory models are used by environmental control agencies to estimate and/or predict the impact of a given pollution emission source(s) on air quality at a downwind receptor site(s). The Environmental Protection Agencies of the United States and Canada are working to improve the predictive capabilities of long distance transport dispersion models by incorporating new procedures to take into consideration such factors as transformation mechanisms of gases to aerosols ($SO_2 \rightarrow SO_4$) and deposition of those species enroute between source and receptor over distances of 10^2 km and 10^3 km. These transport or trajectory models are under development principally to assist the U. S. Environmental Protection Agency in understanding the mechanisms of transport of acid gases and aerosols in order to aid in calculating the effect of differing types of emission control strategies on regional air quality. These new models typically take into consideration advective motion of the atmosphere, dispersion caused by atmospheric turbulence and the impact of pollutant removal mechanisms resulting from the pollutant mixing with clouds and wet and dry deposition processes.

These types of dispersion models require a considerable amount of emission inventory data and meteorological information and a computer capable of performing the computations. Often the computations are expensive because a substantial amount of computer time is required to perform the computations.

Recently several groups have been examining complementary modeling procedures which combine atmospheric dispersion data with source and air quality measurements into a hybrid receptor modeling procedure. This report discusses and compares two of these hybrid receptor modeling approaches to calculate the impact of pollutants emitted from electric power generating facilities burning fossil fuel on downwind receptor sites.

For the purpose of this presentation we have defined a hybrid receptor model(Stevens and Pace, 1984) as any procedure which makes use of both receptor and dispersion modeling principles to calculate the impact of primary pollutant emissions on a downwind receptor site.

A receptor model uses the ambient air chemistry data collected at a receptor site and information on the chemical characteristics of nearby major emission sources to calculate the impact of these sources on the receptor site.

2. DISCUSSION

Diffusion Hybrid Receptor Model A steady state two-dimensional model has been developed by Fay and Rosenzweig (1980), which estimates the ambient pollutant concentrations of SO_4 at a receptor site originating from distant sources (> 100 km) and averaged over long periods (e.g. month, season or year).

The Fay and Rosenzweig model may be expressed as shown in equation (1)

$$C'_k = \sum_j R_{kj} Q_j \qquad (1)$$

where C'_k (C_k) = predicted (or measured) concentration of secondary pollutant (SO_4) at receptor site K;

Q_j = emission rate of primary pollutant(SO_2) for source j (known);

R_{kj} = SO_4 transfer coefficient from source j to receptor site k.

R_{kj} value is obtained by solving a steady state, time-averaged, two dimensional Eulerian diffusion equation where R_{kj} is a complex function of 9 unknowns assumed to be constant throughout the flow field from source to receptor.These unknowns are (1) mixing height,(2) wind speed and (3) direction, (4) horizontal diffusivity, (5)rate constants for the conversion of SO_2 to sulfate, (6) wet and (7) dry deposition, and rate constants for SO_4 (8) wet and (9) dry deposition.

The unknowns are determined by mathematically minimizing the differences between the measured SO_4 (C_k)at a receptor site and the predicted SO_4 (C'_k). Then with the values obtained from the minimization process Fay (1980) found a correlation coefficient of 0.87 between the model predicted concentrations of SO_4 and the SO_4 measured at SURE monitoring sites (Hidy et al. 1978) in the Eastern United States.

Table 1 contains a list of the optimum sulfate dispersion parameters for the Eastern U.S. determined as described above from the Fay (1980) model. These values as can be seen in the table are products of a combination of dispersion values

(e.g., diffusivity D_h) and physical parameters (e.g., wind speed W, and deposition constants τ). The physical parameters selected by Fay (1980) to produce reasonable correlations between observed and predicted sulfate concentrations were also in general agreement with values obtained by previous investigators.

Table 1 Optimum Sulfate Dispersion Parameters for Eastern U.S.

$\tau D_h (m^2)$	1.3×10^{11}
$\tau_s D_h (m^2)$	2.5×10^{11}
$D_h^2/w^2 (m^2)$	4.0×10^{12}
$D_h^2 \tau_c (m^4 s^{-1})$	9.78×10^{17}
Wind Direction	270° True West
Background $SO_4^=$ ($\mu g/m^3$)	5.95

The Fay (1980) model calculations for the annual average concentrations of sulfate formed from U.S. fossil fuel power plant emissions provided excellent correlations with observed ambient measurements. The model has the advantage of not requiring a large computer to perform the computations, but does have the limitation of using data averaged over long time periods. Recently Fay et al. (1986) were able to use this model to predict the three largest contributions to wet $SO_4^=$ deposition in Eastern U.S.: Ohio (11.9%), Pennsylvania (11.4%) and New York (7.8%). The apportionment of airborne sulfate was also accomplished using the same parameter values obtained as described above. This hybrid model has the ability to predict impact of emission reductions of SO_2 on downwind sulfate concentrations. The accuracy of the predictions will be affected by deviations from non-linear transformations and deposition rates assumed in the formulation. Nevertheless, reasonable estimates of the impact of SO_2 emission reductions on downwind receptor areas appear to be achievable by the model.

Tracer Hybrid Receptor Model Lewis and Stevens (1985) have derived a hybrid receptor model to calculate the amount of secondary sulfate that would be formed during transport and arrive at a specified receptor site from an identifiable emission source.

The model is based on the following assumptions:

1. deposition and transformation of the SO_2 to sulfate during transport are first-order processes, but may have complex dependences on time;

2. dispersion of chemical species emitted from the source are identical during transport;

3. dry deposition is the only deposition that occurs;

4. deposition affects all fine particles in an identical manner, but may be different for SO_2; and

5. SO_2 is converted to sulfate by homogeneous gas phase oxidation.

These assumptions lead to the following expressions:

$$M_{SO2} = M_p A(0) \exp [-(\bar{k}_r + \bar{k}_d)t] \quad (2)$$

$$M_{SO4} = 3/2\ M_p A(0) T + M_p B(0) \quad (3)$$

where M_{SO4} is the mass of total sulfate (primary and secondary) that is measured at the receptor site, M_p is the mass concentrations of fine particles from the source (calculated from a classical receptor model), and T, a complex term containing both the transformation of SO_2 to sulfate in transit between source and receptor and losses due to deposition.

The quantities $\bar{k}_r$ and $\bar{k}_d$ are respectively the average transformation rate for SO_2, and the average excess deposition rate for SO_2 in comparison with that of fine particles, during the time of travel t between source and receptor. Finally, A(0) and B(0) are defined as

$$A(0) = \frac{\text{mass emission rate [g s}^{-1}\text{] of SO}_2}{\text{mass emission rate [g s}^{-1}\text{] of primary fine particles}}$$

$$B(0) = \frac{\text{emission rate [g s}^{-1}\text{] of primary SO}_4^=}{\text{mass emission rate [g s}^{-1}\text{] of primary fine particles}}$$

The average transformation/deposition factor T can be approximated (Lewis and Stevens, 1985) by

$$T = \frac{\bar{k}_r}{\bar{k}_r + \bar{k}_d} [1 - \exp ((-\bar{k}_r + \bar{k}_d)\ t)] \quad (4)$$

resulting in a substantial simplification of equation (3).

The calculation of the secondary sulfate is, therefore, the coupling of the emission ratio (SO_2/Tracer species), wind speed and trajectory information, with a conventional receptor modeling solution to calculate the primary impact of the source on the receptor. The key feature of this analytical model is that a large part of the complicating features of dispersion and deposition of the secondary sulfate is implicitly contained in the M_p term, which serves as the tracer for the source.

Gordon and Olmez (1986) have used this approach to model the sulfate resulting from multiple sources in the Ohio Valley. Their results were qualitatively consistent with the measured aerosol S/Se ratio of between 1700 and 3000 measured at receptor sites downwind of the multiple sources (coal-fired power plants).

In August of 1983 a field sampling study was conducted in rural Maryland at a location (Deep Creek Lake) which was anticipated to be heavily impacted by primary and secondary emissions from coal-fired power plants West, Northwest, and Southwest of the monitoring site. The study provided a data base which contains elemental composition obtained by X-ray fluorescence and instrumental neutron activation methods for 130 6-

hour consecutive intervals of size fractionated aerosols. In addition, 6-hour back trajectory meteorological data were obtained along with ambient gas (SO_2, O_3 and NO_x) measurements, source signatures from 3 large power plants west of the receptor site and a regional elemental composition signature collected in western Ohio. Table 2 contains the averages of selected fine particle species and gaseous sulfur measured at Deep Creek Lake monitoring site.

Table 2. Averaged Fine Particle and Gaseous Sulfur Concentrations at Deep Creek Lake, MD

Species	10 am-10 pm ng/m^3	10 pm-10 am ng/m^3
Mass	52,700	39,800
Sp*	8,570	6,630
$SO_4^=$	25,700	19,900
Pb	42.5	46.8
Se	4.9	4.9
Sg**	13,900	15,800
Sg/Sp	1.8	3.3

* Fine Particle Sulfur
** Gaseous Sulfur (from SO_2)

Substantial fine mass loadings were prevalent during the study with sulfate representing almost half the total mass. Selenium, which is regarded as a good tracer for coal combustion, correlated as expected with the $SO_4^=$, H^+ and NH_4^+ concentrations (Stevens et al., 1983). The concentration of lead (Pb), traditionally has been a good indicator of mobile source emissions. This study shows the minimal impact on the fine particle mass. Table 3 shows the linear correlation coefficients of the species from Table 2. For 95 six-hour observations a correlation of greater than 0.26 is significant at the 1% level. Thus, the correlations involving lead and the other species are not significant, while the mutual correlations between the gaseous Sg and other species are significant but less so.

Table 3. Linear Correlation Coefficients (N=95)

	Mass	Sp	Sg	Se	Pb
Sp	.94				
Sg	.32	.32			
Se	.75	.73	.40		
Pb	.16	.16	.10	.03	
Sp + Sg	.50	.51	.98	.53	.12

Table 4. Ambient and Source Data for the Fine Particles and Gaseous Sulfur Measurements for the Period August 5, 1983 10am-4pm

	Ambient Date		
Sg	49,300	ng/m^3	(37.6 ppb)
Sp	18,000	ng/m^3	
Se	7.9	ng/m^3	
Sg/Sp	2.7		
Sg/Se	6,240		
Source Data: Ft. Martin Power Plant			
September 1983 $(Sg/Se)_o$	21,000		

Taking Se as tracer (Stevens et al., 1985) for fine particle primary emissions from a single coal-fired power plant upwind of the receptor site, and assuming no primary emissions of sulfate, equations (2) and (3) can be reexpressed as

$$Sp'/Sg' = [\exp((\bar{k}_r + \bar{k}_d)t) - 1]\,\bar{k}_r t/(\bar{k}_r + \bar{k}_d)t \quad (5)$$

$$Sg'/Se' = (Sg/Se)_o \exp[-(\bar{k}_r + \bar{k}_d)t] \quad (6)$$

Sp' is the concentration of sulfate (expressed as sulfur calculated to arrive at the receptor site from an upwind point source.

Sg' and Se' are respectively the concentrations of SO_2 (expressed as sulfur) and fine particle selenium measured at the receptor site and assumed to be from the same single point source (i.e., after background correction). Corresponding source measurements are designated by the subscript (o).

If we assume the primary source of SO_2 and Se measured at our receptor site originates from a single point source (Ft. Martin Power Plant) 45 km west of our site, and the background (Gordon, 1986) of Se' and Sg' (SO_2 expressed as sulfur) to be 2 ng/m^3 and 10 µg/m^3 respectively, then we can calculate the amount of secondary sulfate formed during transport from source to receptor as follows:

We calculate the rate of transformation for data collected on August 5, 1983 using the procedure of Gillani et al. (1981). Based on our O_3 concentrations, estimated solar radiation and mixing height, a value of 2.5%/h for $\bar{k}_r$ was calculated.

Inserting this value and the corrected Sg'/Se' ratio into equation (6) and then solving for $\bar{k}_d$, we find

$$\bar{k}_d = 33\%/h$$

This result also makes use of the 3.2 h transport time derived from back trajectory calculations.

This deposition rate is not unexpected based on the Four Corners Power Plant plume studies of Mamane and Pueschel (1980). In their studies of complex terrain similar to the W.Va.-Md. terrain a deposition of 18% per hour for dry particles was observed. Since dry particles are typically deposited at much lower rates than acidic gases, a 33% h^{-1} excess deposition rate for SO_2 in our experiment does not appear to be unreasonable.

Using the calculated $\bar{k}_d$ and $\bar{k}_r$ values and substituting the data from Table 4 corrected for background concentration of SO_2 into equation (5) we have

$$S_p' = 5900 \text{ ng/m}^3$$

Thus our model estimated that of the 18 $\mu g/m^3$ particle S measured at our Deep Creek Lake receptor site 5.9 $\mu g/m^3$ (33%) is from the conversion of SO_2 to sulfate during transport from the Ft. Martin Plant.

3. CONCLUSIONS

Two types of hybrid models have been described which have the potential of providing cost effective procedures to assess the impact of fossil fuel emission sources on downwind receptor sites and regional air quality. One model developed by Fay and Rosenzweig (1980) incorporates emission data coupled with Eulerian dispersion parameters, chemical transformation constants and deposition rates that are assumed or determined by minimizing the average difference between observed ambient sulfate concentrations and those predicted by the model. This model is most effective at distances > 100 km and periods of seasons The tracer hybrid model uses chemical composition data from the source and receptor and back trajectory data to calculate the secondary sulfate formed during transport.

The tracer model does not require the meteorological dispersion terms since they are implicitly part of the tracer analytical information. Both models assume linear transformation rates and deposition rates which would impact the accuracy of the models depending on the deviation of these values from linearity.

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